

# $\mathbb{Z}_2$ invariant protected bound states in topological insulators

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We present an exact solution of a modified Dirac equation for topological insulator in the presence of a hole or vacancy to demonstrate that vacancies may induce bound states in the band gap of topological insulators. They arise due to the  $\mathbb{Z}_2$  classification of time-reversal invariant insulators, thus are also topologically-protected like the edge states in the quantum spin Hall effect and the surface states in three-dimensional topological insulators. Coexistence of the in-gap bound states and the edge or surface states in topological insulators suggests that imperfections may affect transport properties of topological insulators via additional bound states near the system boundary.

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Topological insulators are narrow-band semiconductors with band inversion generated by strong spin-orbit coupling [1]. They are distinguished from the ordinary band insulators according to the  $\mathbb{Z}_2$  invariant classification of the gapped band insulators due to the time reversal symmetry. The variation of the  $\mathbb{Z}_2$  invariant at their boundaries will lead to the topologically protected edge or surface states with the gapless Dirac energy spectrum[2–7]. Imperfections, such as impurity, vacancy, and disorder, are inevitably present in topological insulators. Owing to the time-reversal symmetry, an exciting feature of topological insulator is that its boundary states are expected to be topologically protected against weak non-magnetic impurities or disorders[8, 9]. This provoked much interest on the single impurity problem on the surface of a topological insulator, starting with gapless Dirac model[10–14]. However, reminding that the boundary state is only a manifestation of the topological nature of the host bulk to know how the imperfections affect the electronic structure. It is well known that single impurity or defect can induce bound states in many systems, such as in the Yu-Shiba state in s-wave superconductor[15, 16] and in d-wave superconductors[17]. Topological defects were discussed in the B-phase of  $^3\text{He}$  superfluid[18] and topological insulators and superconductors [19]. Here we report that bound states can form around a single vacancy in the bulk energy gap of topological insulators. These bound states are found to have the same origin as boundary states due to the  $\mathbb{Z}_2$  classification, thus are also topologically protected.

The formation of the topological bound states can be readily illustrated by reviewing the quantum spin Hall effect in two-dimensional (2D) topological insulators[20–22], in which strong spin-orbit coupling twists the bulk conduction and valence bands, leading to a nontrivial  $\mathbb{Z}_2$  index. As the  $\mathbb{Z}_2$  varies across the edge, edge states arise in the gap with the gapless Dirac dispersion. Unlike the quantum Hall effect in a magnetic field, spin-orbit coupling preserves the time reversal symmetry, so the result-

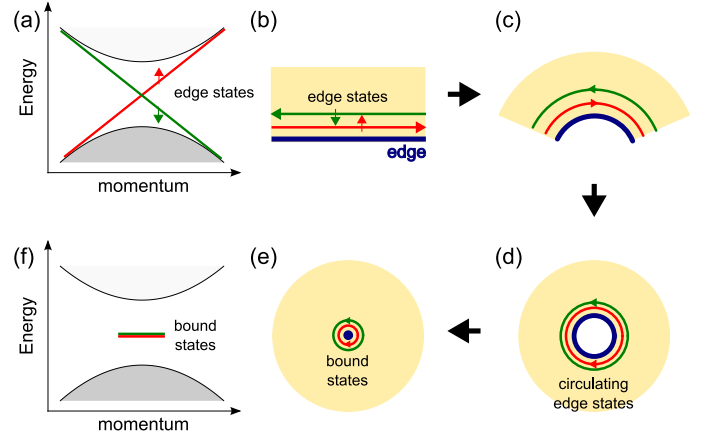


FIG. 1: Schematic description of the formation of vacancy-induced in-gap bound states in two-dimensional topological insulators. [(a) and (b)] A pair of helical edge states traveling along the edge of a 2D topological insulator with the gapless Dirac dispersion. [(c) and (d)] When the edge is bent into a hole, the helical edge states evolve to circulate around the hole. [(e) and (f)] The circulating edge states may develop into topologically-protected bound states as the hole shrinks into a point or being replaced by a vacancy. The same physics is expected to happen in one and three dimensions.

ing edge states appear in helical pairs, in which one state is the time-reversal counterpart of the other, propagating along opposite directions and with opposite spins (Fig. 1). Now imagine that the system edge is rolled into a hole, the edge states will circulate around the hole as the periodic boundary condition along the propagating direction remains unchanged. While shrinking its radius of the hole, most of the edge states will be expelled into the bulk bands as the energy separation of the states becomes larger and larger, and it is found that at least two degenerate pairs of the states will be trapped to form the bound states in the gap while the hole will evolve into a point defect. This mechanism of the formation of the bound states can be realized in topological insulator in all the dimensions.

We will employ a modified Dirac model to provide a unified description of topological insulators in various dimensions

$$H_0 = v\mathbf{p} \cdot \boldsymbol{\alpha} + (mv^2 - Bp^2)\beta. \quad (1)$$

The modification comes from the quadratic correction in momentum  $-Bp^2$  to the band gap  $mv^2$ .  $p_i = -i\hbar\partial_i$  is the momentum operator ( $i \in \{x, y, z\}$ ),  $p^2 = p_x^2 + p_y^2 + p_z^2$ ,  $v$  and  $m$  have the dimension of the speed and mass, respectively.  $B$  has the dimension of  $m^{-1}$ . The Dirac matrices satisfy the anticommutation relations  $\alpha_i\alpha_j = -\alpha_j\alpha_i$  ( $i \neq j$ ),  $\alpha_i\beta = -\beta\alpha_i$  and  $\alpha_i^2 = \beta^2 = 1$ . One representation of the Dirac matrices in three spatial dimensions can be expressed as a set of  $4 \times 4$  matrices

$$\alpha_i = \sigma_x \otimes \sigma_i, \quad \beta = \sigma_z \otimes \sigma_0, \quad (2)$$

where  $\sigma_{i=x,y,z}$  are the Pauli matrices,  $\sigma_0$  is the  $2 \times 2$  unit matrix, and  $\otimes$  represents the Kronecker product. This modified Dirac Hamiltonian preserves the time reversal symmetry  $\hat{\Theta}H_0\hat{\Theta}^{-1} = H_0$  under the time reversal operation  $\hat{\Theta} = -i\alpha_x\alpha_z\hat{K}$ , where  $\hat{K}$  is the complex conjugate operator. This equation has the identical mathematical structure as the effective models for the quantum spin Hall effect and 3D topological insulator[21, 23–25]. It becomes topologically non-trivial if  $mB > 0$ , while topologically trivial if  $mB < 0$  according to the  $\mathbb{Z}_2$  classification of insulators[26, 27]. Due to the bulk-boundary correspondence [28, 29], there always exist topologically protected boundary states at the open boundaries of a topological insulator, where the  $\mathbb{Z}_2$  invariant changes from nontrivial to trivial. This feature can be well described by the modified Dirac model when  $mB > 0$ . Starting from this modified Dirac model, we are now ready to explore existence of the in-gap bound states induced by a single vacancy by presenting an exact solution of the modified Dirac model.

In two dimension ( $p_z = 0$ ) the equation can be reduced into two independent  $2 \times 2$  hamiltonians

$$h_{\pm} = (mv^2 - Bp^2)\sigma_z + \hbar v(p_x\sigma_x \pm p_y\sigma_y), \quad (3)$$

with  $h_-$  the time-reversal counterpart of  $h_+$ , which was already studied in the HgTe quantum well[21], and in the thin films of  $\text{Bi}_2\text{Se}_3$ [24, 25]. It is convenient to adopt polar coordinates  $(x, y) = r(\cos\varphi, \sin\varphi)$  in two dimensions. Here these equations are solved under the vacancy boundary conditions [Fig. 2(a)], i.e., the center of the 2D topological insulator is punched with a hole of radius  $R$ , thus the wavefunction is required to vanish at  $r = R$  and  $r = +\infty$ . Due to the rotational symmetry, the z-component of the total angular momentum  $j_z = -i\hbar\partial_\theta + (\hbar/2)\sigma_z$  provides a good quantum number, labeled by a half-integer  $m_j \in \{\pm 1/2, \pm 3/2, \dots\}$ , which can be used to characterize the bound states. In this way the equation is reduced to a set of 1D radial equations,

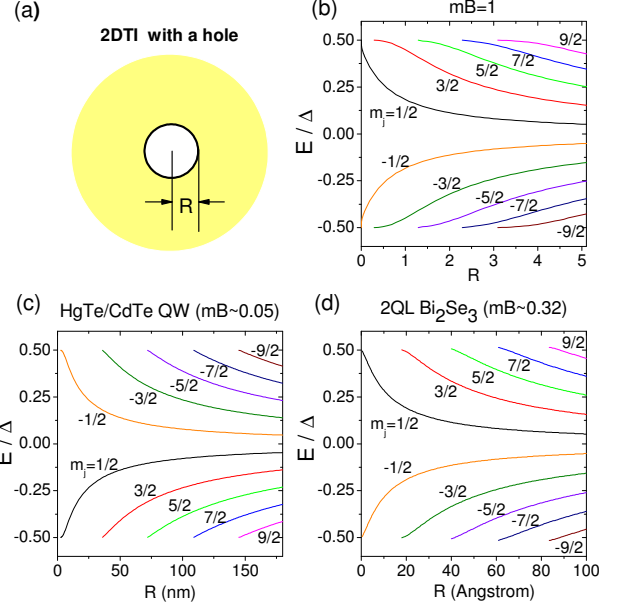


FIG. 2: Two-dimensional topologically protected bound states. (a) A 2D topological insulator with a hole of radius  $R$  at the center. (b)-(c), Energies ( $E$  in units of the band gap  $\Delta$ ) of in-gap bound states circulating around the hole as functions of the hole radius.  $m_j$  is the quantum number for z-component of total angular momentum of the circulating bound states. In (b),  $m = v = B = \hbar = 1$  and  $\Delta = \sqrt{3}$  in (c),  $mv^2 = -10$  meV,  $B\hbar^2 = -686$  meV·nm<sup>2</sup>, and  $\hbar v = 364.5$  meV·nm,  $\Delta = 20$  meV, adopted from Ref. [21]; in (d),  $mv^2 = 0.126$  eV,  $B\hbar^2 = 21.8$  eVÅ<sup>2</sup>,  $\hbar v = 0.294$  eVÅ,  $\Delta = 0.252$  eV, adopted from Ref. [30].

which can be solved exactly. The trial wave function has the form  $(\psi_1, \psi_2)^T e^{\lambda r}$ . The secular equations of the indeterminate coefficients  $(\psi_1, \psi_2)^T$  give four roots of  $\lambda_n$  ( $= \pm\lambda_1, \pm\lambda_2$ ) in terms of the energy  $E$ ,

$$\lambda_{1,2}^2 = \frac{v^2}{2B^2\hbar^2} [1 - 2mB \pm \sqrt{1 - 4mB + 4B^2 E^2 / v^4}]. \quad (4)$$

Using the boundary conditions at  $r = R$  and  $r = +\infty$  we finally arrive at the transcendental equation for the bound state energies

$$\frac{\lambda_1^2 + \frac{mv^2 - E}{B\hbar^2}}{\lambda_1} \frac{K_{m_j + \frac{1}{2}}(\lambda_1 R)}{K_{m_j - \frac{1}{2}}(\lambda_1 R)} = \frac{\lambda_2^2 + \frac{mv^2 - E}{B\hbar^2}}{\lambda_2} \frac{K_{m_j + \frac{1}{2}}(\lambda_2 R)}{K_{m_j - \frac{1}{2}}(\lambda_2 R)}, \quad (5)$$

and the wavefunction  $\Psi_{m_j}(r, \theta)$  for  $h_+$  turns out to have the form

$$\begin{bmatrix} \frac{K_{m_j - \frac{1}{2}}(\lambda_1 R)}{K_{m_j + \frac{1}{2}}(\lambda_1 R)} \left[ \frac{K_{m_j - \frac{1}{2}}(\lambda_1 r)}{K_{m_j - \frac{1}{2}}(\lambda_1 R)} - \frac{K_{m_j - \frac{1}{2}}(\lambda_2 r)}{K_{m_j - \frac{1}{2}}(\lambda_2 R)} \right] e^{i(m_j - \frac{1}{2})\theta} \\ i \frac{\lambda_1^2 + \frac{mv^2 - E}{B\hbar^2}}{(\lambda_1 v / B\hbar)} \left[ \frac{K_{m_j + \frac{1}{2}}(\lambda_1 r)}{K_{m_j + \frac{1}{2}}(\lambda_1 R)} - \frac{K_{m_j + \frac{1}{2}}(\lambda_2 r)}{K_{m_j + \frac{1}{2}}(\lambda_2 R)} \right] e^{i(m_j + \frac{1}{2})\theta} \end{bmatrix}, \quad (6)$$

where  $K_n(x)$  is the modified Bessel function of second kind.

In Fig. 2 (b)-(d), we show the bound-state energies as functions of  $R$  for an ideal case [(b),  $mB = 1$ ], for the HgTe quantum well ( $mB = 0.05$ )[21], and for a 2 quintuple layer thick  $\text{Bi}_2\text{Se}_3$  thin film ( $mB = 0.32$ )[30]. For a macroscopically large  $R$ , we found an approximated solution for the energy spectrum of  $h_+$  as  $E = m_j \hbar v \text{sgn}(B)/R$ . As the time-reversal copy of  $h_+$ ,  $h_-$  has an approximated spectrum  $E = -m_j \hbar v \text{sgn}(B)/R$ . They form a series of paired helical edge states, in good agreement with the edge-state solutions in a 2D quantum spin Hall system [31] if we take  $k = m_j/R$  for a large  $R$ . When shrinking  $R$ , the energy separation of these edge state  $\Delta E = \pm \hbar v / R$  increases with decreasing  $R$ , and the edge states with higher  $m_j$  will be pushed out of the energy gap gradually. However, we observe that for  $mB > 0$  two pairs of states for  $m_j = \pm 1/2$  always stay in the energy gap, and as  $R \rightarrow 0$  their energies approach to  $E = \pm (v^2/2|B|)\sqrt{4mB-1}$  for  $mB > 1/2$  or  $\pm mv^2$  for  $0 < mB < 1/2$ . The solutions demonstrate the formation of the in-gap bound states as illustrated in Fig. 1. Therefore considering the symmetry between  $h_+$  and  $h_-$  we conclude that there always exist *at least* two degenerated pairs of bound states in the energy gap in 2D quantum spin Hall system in the presence of vacancy.

The mechanism of the formation of the in-gap bound states is applicable to 3D topological insulators.[23, 32] In 3D, the modified Dirac equation with a central potential becomes a classical problem, the hydrogen atom-like problem. For the Coulomb potential, it was exactly solved to give the fine structure of light spectra of hydrogen atom. Similarly, the eigenstates of the 3D modified Dirac equation with a central potential can be labeled by three good quantum numbers. The first two are the total angular momentum  $\hat{\mathbf{J}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} + \frac{\hbar}{2}\hat{\Sigma}$  and its  $z$ -component  $\hat{J}_z$ , where the spin operator  $\hat{\Sigma}_\alpha = \sigma_0 \otimes \sigma_\alpha$  ( $\alpha = x, y, z$ ). The eigenvalues of  $\hat{\mathbf{J}}^2$  and  $\hat{J}_z$  are  $j(j+1)\hbar^2$  and  $m_j\hbar$ , respectively, with  $j \in \{\frac{1}{2}, \frac{3}{2}, \dots\}$  and  $m_j \in \{-j, \dots, j\}$ . The third conserved quantity is the spin-orbit operator  $\hat{\kappa} = \beta(\hat{\mathbf{r}} \times \hat{\mathbf{p}} \cdot \hat{\Sigma} + \hbar)$ . Note that  $\hat{\kappa}^2 = \hat{\mathbf{J}}^2 + \hbar^2/4$ , then the eigenvalues of  $\hat{\kappa}$  is  $\hbar\kappa = \pm\hbar(j+1/2) = \pm\hbar, \pm 2\hbar, \dots$ . Thus  $\kappa$  here is similar to the  $\pm$  index in 2D that separate the hamiltonian into  $h_\pm$ . These conserved quantities also help to reduce the problem into a set of 1D radial equations.[33] In the presence of the vacancy or a cavity of radius  $R$  with the boundary conditions at  $\Psi(R) = \Psi(\infty) = 0$ , the radial part of the wave function can be solved in terms of the modified spherical Bessel function of the second kind  $k_n(x)$ . With the help of the recursion relation of  $k_n(x)$ , the transcendental equations for the bound state energies can be found as

$$\frac{\lambda_1^2 + \frac{mv^2-E}{B\hbar^2} k_{j\pm\frac{1}{2}}(\lambda_1 R)}{\lambda_1 k_{j\mp\frac{1}{2}}(\lambda_1 R)} = \frac{\lambda_2^2 + \frac{mv^2-E}{B\hbar^2} k_{j\pm\frac{1}{2}}(\lambda_2 R)}{\lambda_2 k_{j\mp\frac{1}{2}}(\lambda_2 R)} \quad (7)$$

for  $\kappa = j + \frac{1}{2}$  and  $-(j + \frac{1}{2})$ , respectively. The corresponding wavefunction  $\Psi_{j,\kappa}^{m_j}(r, \theta, \phi)$  are of the form

$$\Psi_{j,\kappa}^{m_j}(r, \theta, \phi) \propto \begin{bmatrix} \frac{i(\lambda_1 v/B\hbar)}{\lambda_1^2 + \frac{mv^2-E}{B\hbar^2}} \left[ \frac{k_{j\mp\frac{1}{2}}(\lambda_1 r)}{k_{j\mp\frac{1}{2}}(\lambda_1 R)} - \frac{k_{j\mp\frac{1}{2}}(\lambda_2 r)}{k_{j\mp\frac{1}{2}}(\lambda_2 R)} \right] \phi_{j,m_j}^{A/B} \\ \frac{k_{j\pm\frac{1}{2}}(\lambda_1 r)}{k_{j\mp\frac{1}{2}}(\lambda_1 R)} \left[ \frac{k_{j\pm\frac{1}{2}}(\lambda_1 r)}{k_{j\pm\frac{1}{2}}(\lambda_1 R)} - \frac{k_{j\pm\frac{1}{2}}(\lambda_2 r)}{k_{j\pm\frac{1}{2}}(\lambda_2 R)} \right] \phi_{j,m_j}^{B/A} \end{bmatrix} \quad (8)$$

where

$$\phi_{j,m_j}^A(\theta, \varphi) = \begin{bmatrix} \sqrt{\frac{j+m_j}{2j}} Y_{j-\frac{1}{2}}^{m_j-\frac{1}{2}}(\theta, \varphi) \\ \sqrt{\frac{j-m_j}{2j}} Y_{j-\frac{1}{2}}^{m_j+\frac{1}{2}}(\theta, \varphi) \end{bmatrix}, \quad (9)$$

$$\phi_{j,m_j}^B(\theta, \varphi) = \begin{bmatrix} -\sqrt{\frac{j-m_j+1}{2(j+1)}} Y_{j+\frac{1}{2}}^{m_j-\frac{1}{2}}(\theta, \varphi) \\ \sqrt{\frac{j+m_j+1}{2(j+1)}} Y_{j+\frac{1}{2}}^{m_j+\frac{1}{2}}(\theta, \varphi) \end{bmatrix}, \quad (10)$$

and  $Y_j^m(\theta, \varphi)$  is the spherical harmonics.  $\phi_{j,m_j}^A$  and  $\phi_{j,m_j}^B$  possess opposite parities.

Although the rotational symmetry simplifies the problem, it is believed that the presence of the bound states is not sensitive to the shape of the vacancy, because of their topological origin. As an example we choose a set of parameters based on first principles calculations for  $\text{Bi}_2\text{Se}_3$  by ignoring the anisotropy, where  $mv^2 = 0.28\text{eV}$ ,  $\hbar v = 3.2\text{eV}\text{\AA}$ , and  $B = 33\text{eV}\text{\AA}^2$ . In this case  $mB \sim 1 > 1/2$ . Similar to the 2D case, we find that the surface states around the cavity exist for a large radius  $R$  as expected by the bulk-boundary correspondence for a  $\mathbb{Z}_2$  invariant topological insulators[29]. The states with larger orbital angular momentum are eventually expelled into the bulk band while the radius is shrinking. We plot several bound state energies of small orbital angular momenta as a function of the radius  $R$  in Fig. 3. For convenience, the bound states are labeled by the quantum number  $\kappa$  for the spin-orbit operator. Each  $\kappa$  corresponds to  $(2j+1)$ -fold degenerate states of different  $m_j$ . Note that when the vacancy radius is only several angstroms, two degenerate pairs of bound-state energies can survive. Detailed analysis of the solution indicates that the spatial distribution of a bound state is comparable with that of the edge or surface states (for a large  $R$  in the present case), which are determined by the model parameters and slightly depends on  $R$ . From the evolution of the edge or surface states into the in-gap bound states, we think their formation have the same topological origin. Thus these in-gap bound states are also protected topologically as the edge or surface states.

Now we come to address possible implication of these solutions to topological insulators. Due to the overlapping in energy, when the vacancies or defects are located close to the boundary, the induced in-gap bound states may sabotage the electronic transport through the boundary states. When the wave functions of the in-gap bound state and the edge or surface states overlaps in the space, the distortion of the wave functions of these

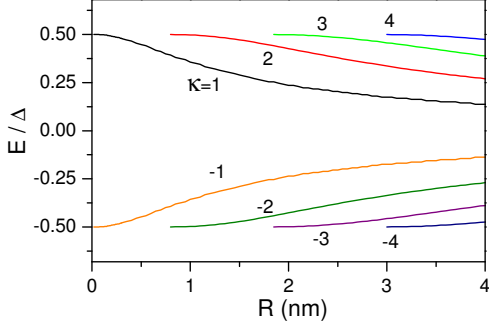


FIG. 3: Three-dimensional topologically protected bound states. Energies ( $E$  in units of the band gap  $\Delta$ ) of in-gap bound states covering a vacancy in a 3D topological insulator as functions of the vacancy radius  $R$ .  $\kappa$  is the quantum number of the spin-orbit operator. Parameters:  $mv^2 = 0.28\text{eV}$ ,  $\hbar v = 3.2\text{eV}\text{\AA}$ , and  $B\hbar^2 = 33\text{eV}\text{\AA}^2$ .  $mB = 0.90$  and  $\Delta = 0.50\text{eV}$ .

states due to the boundary conditions will cause the energy change in these states. As a result, we may also regard that there exists a transition amplitude between these states. For example, in the 2D quantum spin Hall system, there exists a pair of helical edge states with a linear dispersion,  $E_{k,\pm} = \pm\hbar vk$ . Consider a vacancy or defect appears near the boundary. The effective model for a pair of helical edge states in the presence of the defect states has the form,

$$H = \sum_{k,\sigma=\pm} \hbar vk \sigma c_{k\sigma}^\dagger c_{k\sigma} + \sum_n \epsilon_n d_n^\dagger d_n + \sum_{k,\sigma,n} (T_{k\sigma}^n c_{k\sigma}^\dagger d_n + h.c.)$$

where  $c_{k\sigma}^\dagger$  and  $c_{k\sigma}$  are the creation and annihilation operators of edge states and  $d_n^\dagger$  and  $d_n$  are for the  $n$ th in-gap bound states with the energy  $\epsilon_n$ . The resulting dispersions for the edge states are no longer linear in the momentum, and open energy gaps  $\Delta E = 2|T_{k\sigma}^n|$  at the resonant point  $\epsilon_n = \hbar vk\sigma$ .  $T_{k\sigma}^n$  is a function of the relative position between the defect or vacancy and the boundary. In the HgTe/CdTe quantum wells, a typical size of the edge states and bound states is about 50 - 100 nm. The energy gap opening here is *not* caused by breaking the time reversal symmetry. The mechanism is similar to the finite size effect in the quantum spin Hall system, where the overlap of the edge states living on opposite edges causes an energy gap[31]. In that case the energy splitting is about 0.5 meV for a strip system with a width of 200 nm. The effect is large enough to be measured experimentally. This may help to understand why the non-zero conductance is narrowed to a small region of gate voltage in the HgTe/CdTe quantum wells[22]. The in-gap bound states may also be one of the possible mechanisms for the low mobility in 3D topological insulators.

However, blessings usually come in disguise. The whole semiconductor business depends on how the positive and

negative effects of impurities and vacancies are precisely balanced. The topologically-protected bound states for sure are essentially different from those we know before, as they are subjected to some topological nature and confined to a mesoscopic scale. Their possible impact and applications for topological insulators in future deserve further studies to explore.

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